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An Annotated Bibliography on Proton Affinities

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Institute for Materials Research
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Final

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Prepared for
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U.S. DEPARTMENT OF COMMERCE, Elliot L. Richardson, *Secretary*

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An Annotated Bibliography on Proton Affinities

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Abstract

This bibliography consists of approximately 150 references about proton affinities which cover the period from 1932 through 1975. Included are experimental determinations of proton affinities in the gas phase (through observation of proton transfer reactions, ion-molecule equilibria, and appearance potential measurements) as well as determinations from crystal lattice energies and other miscellaneous techniques. Also included are reviews concerned with or related to proton affinity determinations.

Key words: Appearance potential; basicity; bibliography; heat of formation; ion-molecule equilibrium; proton affinity; proton transfer

Introduction

During the past twenty years, major advances have been made in the understanding of the chemical reactions of ions in the gas phase. An important outgrowth of this work is a growing body of information about gas phase acidities and basicities. The scale of gas phase basicities is usually quantified in terms of the proton affinities of the molecules. The proton affinity is defined as the negative of the enthalpy change resulting from the addition of a proton to a base to form the conjugate acid. This definition was originally formulated to express the basicities of molecules in solution.

This field of research has developed to the point that areas of potential scientific usefulness are becoming defined. For example, the scale of gas phase basicities is now being used as a reference scale against which to examine, define, and ultimately understand and control solvent effects on chemical equilibria and reactivity. A practical application of the proton affinity scale is its usefulness for selecting appropriate reagent gases for use in the analytical application of ion-molecule reactions known as "chemical ionization mass spectrometry" which is finding widespread application in biochemical and biomedical studies. Finally, through proton affinity measurements there now exists ion thermochemical information which ultimately must be brought into accord and combined with the much larger body of ion thermochemical information derived from spectroscopic and appearance potential measurements. In fact, this new body of proton affinity measurements imparts for the first time a network character to ion thermochemical information, thus posing opportunities for searching tests of the accuracy of various experimental measurements and their interpretation in terms of thermochemical quantities.

Scope of Bibliography

This bibliography is intended to cover the literature concerned with gas phase proton affinities of neutral molecules from the earliest papers on the subject until the cut-off date of December 31, 1975.

In principle, there are two ways to define the scope of a bibliography on proton affinities. One could include every paper whose results directly or indirectly give information which can be related to proton affinities, even though the authors did not specifically interpret their results in those terms. Alternatively, one can simply limit the bibliography to work which specifically concerns itself with proton affinities. We have chosen the latter course even though in doing so we may be neglecting to mention certain studies which contribute useful data. The user of this compilation will be able to locate pertinent related data through the references listed in the papers of the bibliography. To include all of these related papers in the bibliography itself would mean including a large fraction of the literature on appearance potential measurements of hydrogen-containing ions. A separate comprehensive compilation of these measurements will appear shortly. Many of these articles would be of only peripheral interest to the subject of proton affinities.

We also include a list of review articles and papers which discuss factors relating to proton affinities. Theoretical calculations are not included.

Presentation of Bibliography

The main body of the bibliography consists of a numbered list of papers, subdivided into five categories. These are: (X) experimental determinations of proton affinities based on ion-equilibrium measurements, or

limits on proton affinities based on the occurrence (or non-occurrence) of ion-molecule reactions, or on determinations of crystal lattice energies; (Y) experimental determinations of proton affinities based on appearance potential measurements; (Z) experimental determinations of proton affinities through miscellaneous approaches unrelated to those of the first two categories; (O) derivations of proton affinities through empirical relationships to other quantities such as ionization potentials or core electron binding energies; (R) selected reviews and papers which present related and background information.

For each paper we list the molecules corresponding to the proton affinities determined in that paper. In cases where bracketing techniques or proton transfer equilibria are used to generate proton affinities, we list not only the species whose proton affinity has been determined, but also the reference molecules.

In addition, we present a list sorted according to chemical species. Here again, we give both the molecule whose proton affinity is determined and any reference species used in the determination. The order of presentation of the molecules is that of increasing atomic number and molecular complexity.

An author index is also included.

Literature Search

Literature references were obtained initially both by a computer search for Chemical Abstracts entries on proton affinities going back to 1970, and also by an issue-by-issue search of the following major journals, going back to 1960:

Journal of Chemical Physics
Journal of Physical Chemistry
Journal of the American Chemical Society
Journal of Research of the National Bureau of Standards
The International Journal of Mass Spectrometry and Ion Physics
International Journal of Chemical Kinetics
Canadian Journal of Chemistry
Chemical Physics Letters
Transactions of the Faraday Society

Additional entries were found by cross-referencing articles referred to in reviews and papers of interest.

Acknowledgements

We are grateful to Mrs. Candyce L. Schmidt for her skillful assistance in all phases of the preparation of this document, to Mr. K. Draxl and Mr. J. G. Koch who provided helpful information on searching and document preparation, to Dr. L. W. Sieck for his assistance in the literature search, and to Dr. G. W. A. Milne of the National Institutes of Health for his help and encouragement.

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X1 - 72 Chong, S. L., Myers, R. A. Jr., and Franklin, J. L.,
 Proton Affinity of Water, J. Chem. Phys. 56, 2427 (1972).

H₂O, HCOOH, D₂S, H₂S

X2 - 73 Cotter, R. J., and Koski, W. S., Reaction of D₃O⁺ with
 D₂: Proton Affinity of Water, J. Chem. Phys. 59,
 784 (1973).

D₂O, H₂O

X3 - 70 Long, J., and Munson, B., On the Proton Affinity of Water,
 J. Chem. Phys. 53, 1356 (1970).

H₂O, C₃H₆, cis-2-C₄H₈, (CH₃)₂CH, HCH₃, C₂H₄, CH₃SH

X4 - 69 DePaz, M., Leventhal, J. J., and Friedman, L., Tandem
 Mass-Spectrometer Study of D₃O⁺ and Solvated Derivatives
 J. Chem. Phys. 51, 3748 (1969).

D₂O, H₂O

X5 - 69 Holtz, D., and Beauchamp, J. L., Relative Basicity of Phosphine
 and Ammonia in the Gas Phase, J. Am. Chem. Soc. 91, 5913
(1969).

NH₃, PH₃, (CH₃)₂CH, CH₃CH₃, H₂O, C₂H₄, CH₄

X6 - 71 Roche, A. E., Sutton, M. M., Bohme, D. K., and Schiff, H. I.,
 Determination of Proton Affinity from the Kinetics of
 Proton Transfer Reactions. I. Relative Proton Affinities,
 J. Chem. Phys. 55, 5480 (1971).

CO, N₂O, CH₄, CO₂, CF₄, NO, N₂, H₂, O₂, Ar

X7 - 73 Hemsworth, R. S., Rundle, H. W., Bohme, D. K., Schiff, H. I.,
 Dunkin, D. B., and Fehsenfeld, F. C.,
 Determination of Proton Affinity from the Kinetics
 of Proton Transfer Reactions. III. The Measurement of the

Equilibrium Constant at Various Temperatures, J. Chem. Phys. 59, 61 (1973).

CH₄, CO₂, CO, N₂O

X8 - 71

Chupka, W. A., and Berkowitz, J., Photoionization of Methane: Ionization Potential and Proton Affinity of CH₄, J. Chem. Phys. 54, 4256 (1971).

CH₄

X9 - 65

Munson, M. S. B., and Field, F. H., Reactions of Gaseous Ions. XV. Methane + 1% Ethane and Methane + 1% Propane, J. Am. Chem. Soc. 87, 3294 (1965).

CH₄, C₂H₆

X10 - 57

Lampe, F. W., and Field, F. H., Reactions of Gaseous Ions. III. Formation of Protonated Methane, J. Am. Chem. Soc. 79, 4244 (1957).

CH₄

X11 - 58

Tal'Rose, V. L., and Frankevitch, E. L., Determination of Proton Affinity and Bond Dissociation Energy by Ion Impact Method, J. Am. Chem. Soc. 80, 2344 (1958).

H₂O, CH₃OH, C₂H₅OH, H₂, CH₄, C₂H₆, C₃H₈, C₂H₄, C₃H₆

X12 - 69

Haney, M. A., and Franklin, J. L., Mass Spectrometric Determination of the Proton Affinities of Various Molecules, J. Phys. Chem. 73, 4328 (1969).

CH₃NH₂, NH₃, (CH₃)₂CO, (CH₃)₂O, PH₃, CH₃CN, CH₃SH, CH₃CH₂O, C₆H₆ (Benzene), CH₃OH, HCOOH, HCN, H₂S, HCHO, H₂O, CH₃Cl, HI, CO, HCl, HBr, CH₄

X13 - 72

Cotter, R. J., Rozett, R. W., and Koski, W. S., Reactions of H₂O⁺ and D₂O⁺ with Molecular Hydrogen. I. Proton Affinity of Hydrogen, J. Chem. Phys. 57, 4100 (1972).

H₂, D₂

X14 - 73 Harris, H. H., Crowley, M. G., Grossheim, T. R., Woessner, P. J., and Leventhal, J. J., Binding Energy of H_3^+ , J. Chem. Phys. 59, 6181 (1973).

H₂, D₂

X15 - 68 Leventhal, J. J., and Friedman, L., Experimental Determination of D_3^+ Dissociation Energy, J. Chem. Phys. 49, 1974 (1968).

D₂

X16 - 75 Ridge, D. P., Gas Phase Proton Affinities of Several Fluoroethylenes, J. Am. Chem. Soc. 97, 5670 (1975).

C₂H₃F, CH₂=CF₂, cis-CHF=CHF, trans-CHF=CHF, C₂HF₃, H₂O, H₂S, C₂H₅I, CH₃OH, C₂H₄, CD₃Cl, C₂H₅F, HCHO

X17 - 73 Fennelly, P. F., Hemsworth, R. S., Schiff, H. I., and Bohme, D. K., Determination of the Proton Affinity from the Kinetics of Proton Transfer Reactions. IV. The Equilibrium $O_2H^+ + H_2 = H_3^+ + O_2$ and the Relative Proton Affinity of O₂ and H₂, J. Chem. Phys. 59, 6405 (1973).

O₂, H₂

X18 - 68 Beauchamp, J. L., and Buttrill, S. E., Jr., Proton Affinities of H₂S and H₂O, J. Chem. Phys. 48, 1783 (1968).

H₂S, H₂O, C₂H₄, CO, C₂H₅OH

X19 - 58 Field, F. H., and Lampe, F. W., Reactions of Gaseous Ions. V. Methane-Hydrogen Chloride and Methane-Hydrogen Sulfide, J. Am. Chem. Soc. 80, 5583 (1958).

HCl, H₂S

X20 - 73 Hopkins, J. M., and Bone, L. I., Relative Proton Affinities of Hydrogen Sulfide and Water, J. Chem. Phys. 58, 1473 (1973).

H₂O, H₂S

X21 - 74 Wei, L. Y., and Bone, L. I., Ion-Molecule Reactions

in Methanol and Hydrogen Sulfide, *J. Phys. Chem.*
78, 2527 (1974).

CH_3SH , H_2S

X22 - 68 **Chupka, W. A., and Russell, M. E., Ion-Molecule Reactions of NH_3^+ by Photoionization, *J. Chem. Phys.* 48, 1527 (1968).**

NH_3 , H_2O

X23 - 68 **Chupka, W. A., Russell, M. E., and Refaey, K., Ion-Molecule and Chemi-ionization Reactions in H_2 by Photoionization, *J. Chem. Phys.* 48, 1518 (1968).**

H_2

X24 - 71 **Beauchamp, J. L., Ion Cyclotron Resonance Spectroscopy, *Ann. Rev. Phys. Chem.* 22, 527 (1971).**

CH_4 , SiH_4 , AsH_3 , HF , He , Ne , Ar , Kr , Xe , C_2H_4 , C_3H_6 , $\text{trans-2-C}_4\text{H}_8$, $\text{cis-2-C}_4\text{H}_8$, $\text{1-C}_4\text{H}_8$, $\text{iso-C}_4\text{H}_8$, HCH_3 , CH_3CH_3 , $\text{C}_2\text{H}_5\text{CH}_3$, $(\text{CH}_3)_2\text{CH}_3$, CH_3SH , $\text{C}_2\text{H}_5\text{SH}$, $(\text{CH}_3)_2\text{O}$, $(\text{C}_2\text{H}_5)_2\text{O}$, $(\text{CH}_2)_2\text{O}$ (1,2-Epoxyethane), $(\text{CH}_2)_3\text{O}$ (1,3-Epoxypropane), CH_3SH , $(\text{CH}_3)_2\text{S}$

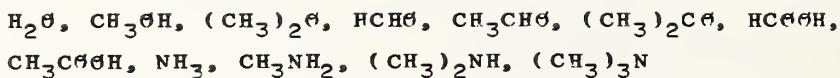
X25 - 71 **Foster, M. S., and Beauchamp, J. L., Potential of Ion Cyclotron Resonance Spectroscopy for the Study of the Intrinsic Properties and Reactivity of Transition Metal Complexes in the Gas Phase. Ion-Molecule Reactions of Iron Pentacarbonyl, *J. Am. Chem. Soc.* 93, 4924 (1971).**

NH_3 , $\text{Fe}(\text{CO})_5$, H_2O , HCl

X26 - 41 **Russell, A. S., Fontana, C. M., and Simons, J. H., Low Velocity Hydrogen Ion Scattering in Hydrogen, Water and Ammonia, *J. Chem. Phys.* 9, 381 (1941).**

H_2 , NH_3

X27 - 65 **Munson, M. S. B., Proton Affinities and the Methyl Inductive Effect, *J. Am. Chem. Soc.* 87, 2332 (1965).**



X28 - 70 Burt, J. A., Dunn, J. L., McEwan, M. J., Sutton, M. M., Roche, A. E., and Schiff, H. I., Some Ion-Molecule Reactions of H_3^+ and the Proton Affinity of H_2 , *J. Chem. Phys.* 52, 6062 (1970).

$\text{H}_2, \theta_2, \text{N}_2, \text{C}\theta_2$

X29 - 72 Beauchamp, J. L., Holtz, D., Woodgate, S. D., and Patt, S. L., Thermochemical Properties and Ion-Molecule Reactions of the Alkyl Halides in the Gas Phase by Ion Cyclotron Resonance Spectroscopy, *J. Am. Chem. Soc.* 94, 2798 (1972).

$\text{C}_3\text{H}_6, \text{C}_2\text{H}_5\text{I}, \text{CH}_3\text{I}, \text{H}_2\text{S}, \text{C}_2\text{H}_5\text{Br}, \text{C}_2\text{H}_5\text{Cl}, \text{H}_2\theta, \text{C}_2\text{H}_5\text{F}, \text{CH}_3\text{Br}, \text{C}_2\text{H}_4, \text{CH}_3\text{Cl}, \text{C}_2\text{H}_2, \text{CH}_3\text{F}, \text{C}\theta, \text{HCl}$

X30 - 75 Pierce, R. C., and Porter, R. F., Ion-Molecule Chemistry of BF_3 and HBF_2 in Hydrogen, *Inorg. Chem.* 14, 1087 (1975).

$\text{BHF}_2, \text{BF}_3, \text{CH}_4, \text{H}_2$

X31 - 70 Kriemler, P., and Buttrill, S. E., Jr., Positive and Negative Ion-Molecule Reactions and the Proton Affinity of Ethyl Nitrate, *J. Am. Chem. Soc.* 92, 1123 (1970).

$\text{C}_2\text{H}_5\theta\text{N}\theta_2, \text{C}_6\text{H}_{10} \text{ (Cyclohexene)}, \text{CH}_3\text{N}\theta_2$

X32 - 74 Goldenfeld, I. V., Korostyshevsky, I. Z., and Mischanchuk, B. G., Analysis of Field Ion Energies in a Mass Spectrometer, *Int. J. Mass Spectrom. Ion Phys.* 13, 297 (1974).

$\text{H}_2\theta, \text{H}_2\text{S}, \text{NH}_3, \text{HC}\theta\theta\text{H}$

X33 - 75 Wilson, M. S., and McCloskey, J. A., Chemical Ionization Mass Spectrometry of Nucleosides. Mechanisms of Ion Formation and Estimations of Proton Affinity, *J. Am. Chem. Soc.* 97, 3436 (1975).

$\text{C}_4\text{H}_4\text{N}_3\theta\text{C}_5\text{H}_9\theta_4 \text{ (Cytidine)}, \text{C}_5\text{H}_3\text{N}_4\text{C}_5\text{H}_9\theta_4 \text{ (9-}\beta\text{-D-Ribose-}$

furanosylpurine), $C_5H_4N_5C_5H_9\theta_4$ (Adenosine), $C_5H_4N_5\theta C_8H_{13}\theta_4$ (2',3'-θ-Isopropylidene guanosine), $C_4H_3N_2\theta_2C_5H_9\theta_4$ (Uridine), $C_5H_5N_2\theta_2C_5H_9\theta_3$ (Thymidine), $C_4H_5N_2\theta_2C_5H_9\theta_4$ (5,6-Dihydrouridine), $C_4H_3N_2\theta_2C_8H_{13}\theta_4$ (2',3'-θ-Isopropylidene uridine), $C_{10}H_{13}N_5$ (6-Amino-9-cyclopentylpurine), $C_6H_7N_5\theta$ (8-Methylguanine), $C_4H_5N_3\theta$ (Cytosine), $C_6H_6N_4$ (6-Methylpurine), $C_5H_5N_5$ (6-Aminopurine), $C_5H_5N_5\theta$ (Guanine), $C_4H_4N_2S_2$ (Dithiouracil), $C_5H_4N_4$ (Purine), $C_5H_4N_4\theta$ (Hypoxanthine) $C_4H_3N_2\theta H$ (2-Hydroxy-1,3-diazine), $C_5H_6N_2\theta_2$ (Thymine), $C_4H_4N_2\theta_2$ (Uracil), $C_5H_3N_4Cl$ (6-Chloropurine), $(CH_3)_2NH$, $(CH_3)_3N$, NH_3 , CH_3NH_2

X34 - 73

Long, J., and Munson, B., Proton Affinities of Some Oxygenated Compounds, *J. Am. Chem. Soc.* 95, 2427 (1973).

NH_3 , $CH_3C\theta\theta CH_2CH_2CH_3$, $C_2H_5C\theta\theta CH_3$, $CH_3C\theta\theta C_2H_5$, $CH_3C\theta\theta CH_3$, $(CH_3)_2C\theta$, $CH_2=C\theta$, $HC\theta\theta CH_2CH_2CH_3$, iso- C_4H_8 , $HC\theta\theta C_2H_5$, tert- $C_4H_9\theta H$, iso- $C_5H_{10}\theta H$, iso- $C_3H_7\theta H$, $(CH_3)_2\theta$, $n-C_3H_7\theta H$, $HC\theta\theta CH_3$, $CH_3CH\theta$, $CH_3C\theta\theta H$, $C_2H_5\theta H$, $CH_3\theta H$, $HC\theta\theta H$, H_2S , $CF_3C\theta\theta H$, $HCH\theta$, $H_2\theta$, C_2H_4 , CH_3Cl , $(C_2H_5)_2\theta$

X35 - 68

Gray, G. A., Study of Ion-Molecule Reactions and Reaction Mechanisms in Acetonitrile by Ion Cyclotron Resonance, *J. Am. Chem. Soc.* 90, 6002 (1968).

CH_3CN , N_2 , HCN , $CH_3\theta H$, $CH_3CH\theta$, $(CH_3)_2C\theta$, $(C_2H_5)_2\theta$

X36 - 69

Searles, S. K., Džidić, I., and Kebarle, P., Proton Affinities of the Alkali Hydroxides, *J. Am. Chem. Soc.* 91, 2810 (1969).

$Li\theta H$, $Na\theta H$, $K\theta H$, $Cs\theta H$

X37 - 70

Holtz, D., Beauchamp, J. L., and Eyler, J. R., Acidity, Basicity, and Ion-Molecule Reactions of Phosphine in the Gas Phase by Ion Cyclotron Resonance Spectroscopy, *J. Am. Chem. Soc.* 92, 7045 (1970).

PH_3 , $H_2\theta$, NH_3 , C_2H_4 , CH_4 , $CH_3CH\theta$, $(CH_3)_2C\theta$

X38 - 70

McDaniel, D. H., Coffman, N. B., and Strong, J. M., Proton Affinity of Trimethylphosphine, *J. Am. Chem.*

$(C_2H_5)_3N$, $(CH_3)_3P$, $(CH_3)_3N$, $(CH_3)_2NH$, NH_3 , PH_3

X39 - 72

Foster, M. S., and Beauchamp, J. L., Gas-Phase Ion Chemistry of Azomethane by Ion Cyclotron Resonance Spectroscopy, J. Am. Chem. Soc. 94, 2425 (1972).

NH_3 , CH_2N_2 (Diazomethane), trans- $CH_3N=NCH_3$, CH_3NH_2

X40 - 72

McAdoo, D. J., McLafferty, F. W., and Bente, P. F., III, Ion Cyclotron Resonance Spectroscopy in Structure Determination. II. Propyl Ions, J. Am. Chem. Soc. 94, 2027 (1972).

C_3H_6 (Cyclopropane), CH_3^6H , H_2S

X41 - 72

Solomon, J. J., and Porter, R. F., Chemical Ionization Mass Spectrometry of Selected Boron Hydrides, J. Am. Chem. Soc. 94, 1443 (1972).

B_2H_6 , B_4H_8 , B_5H_9 , B_5D_9 , B_5H_{11} , B_6H_{10} , C_3H_6 , 1- C_4H_8 , H_2S , H_2^6 , C_2H_4 , CH_4 , C_3D_6 , C_3H_4 , $(CH_3)_2C^6$

X42 - 71

Brauman, J. I., Riveros, J. M., and Blair, L. K., Gas-Phase Basicities of Amines, J. Am. Chem. Soc. 93, 3914 (1971).

tert- $C_4H_9NH_2$, neo- $C_5H_{11}NH_2$, iso- $C_3H_7NH_2$, n- $C_3H_7NH_2$, $C_2H_5NH_2$, CH_3NH_2 , NH_3 , $(C_2H_5)_2NH$, $(CH_3)_2NH$, $(C_2H_5)_3N$, $(CH_3)_3N$

X43 - 71

Bowers, M. T., Aue, D. H., and Webb, H. M., Equilibrium Constants for Gas-Phase Ionic Reactions. Accurate Determination of Relative Proton Affinities, J. Am. Chem. Soc. 93, 4314 (1971).

$(CH_2)_5NH$ (Piperidine), $(CH_3)_3N$, $(CH_2)_4NH$ (Pyrrolidine), $(CH_2)_3NH$ (Trimethylenimine)

X44 - 75

Foster, M. S., and Beauchamp, J. L., Proton Affinity and Gas-Phase Ion Chemistry of Hydrogen Fluoride, Inorg. Chem. 14, 1229 (1975).

HF, N₂, C₂H₂, CH₄

X45 - 72

Chong, S. L., and Franklin, J. L., Proton Affinities of Benzene, Toluene, and the Xylenes, J. Am. Chem. Soc. 94, 6630 (1972).

C₆H₆ (Benzene), C₆H₅CH₃ (Toluene), C₆H₄(CH₃)₂ (1,4-Dimethylbenzene), C₆H₄(CH₃)₂ (1,2-Dimethylbenzene), C₆H₄(CH₃)₂ (1,3-Dimethylbenzene), HCOOH, CH₃SH, (CH₃)₂O, CH₃OH, C₄H₄O (Furan)

X46 - 72

Chong, S. L., and Franklin, J. L., Heats of Formation of Protonated Cyclopropane, Methylcyclopropane, and Ethane, J. Am. Chem. Soc. 94, 6347 (1972).

C₃H₆, CH₃O₂H, HCOOH, C₃H₆ (Cyclopropane), trans-2-C₄H₈, C₃H₅CH₃ (Methylcyclopropane), C₂H₆

X47 - 72

Briggs, J. P., Yamdagni, R., and Kebarle, P., Intrinsic Basicities of Ammonia, Methylamines, Anilines, and Pyridine from Gas-Phase Proton-Exchange Equilibria, J. Am. Chem. Soc. 94, 5128 (1972).

NH₃, CH₃NH₂, (CH₃)₂NH, (CH₃)₃N, C₆H₅NHCH₃ (N-Methylaniline), C₅H₅N (Pyridine), C₆H₅NH₂ (Aniline)

X48 - 72

Aue, D. H., Webb, H. M., and Bowers, M. T., Quantitative Relative Gas-Phase Basicities of Alkylamines. Correlation with Solution Basicity, J. Am. Chem. Soc. 94, 4726 (1972).

NH₃, CH₃NH₂, C₂H₅NH₂, n-C₃H₇NH₂, n-C₄H₉NH₂, iso-C₄H₉NH₂, iso-C₃H₇NH₂, sec-C₄H₉NH₂, tert-C₄H₉NH₂, (CH₃)₂NH, (C₂H₅)₂NH, (n-C₃H₇)₂NH, (n-C₄H₉)₂NH, (iso-C₃H₇)₂NH, (CH₃)₃N, (C₂H₅)₃N, (n-C₃H₇)₃N

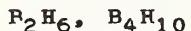
X49 - 73

Kriemler, P., and Buttrill, S. E., Jr., Ion-Molecule Reactions and the Proton Affinities of the Nitroalkanes. I. Nitromethane and Nitroethane, J. Am. Chem. Soc. 95, 1365 (1973).

CH₃NO₂, (CH₃)₂CO, CH₃CH₂O, CH₃CN, C₂H₅OH, C₂H₅CH₂O, C₂H₅NO₂, C₃H₆, H₂S, CH₃OH, C₂H₅NO₂

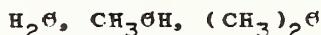
X50 - 73

Pierce, R. C., and Porter, R. F., Low-Temperature
Chemical Ionization Mass Spectrometry of Boron Hydrides.
The Proton Affinities of Diborane and Tetraborane(10),
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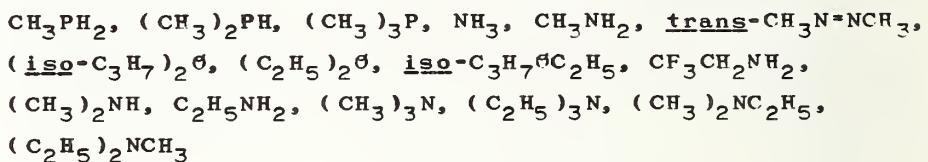
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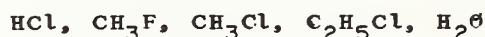
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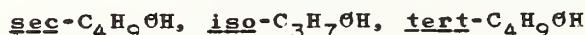
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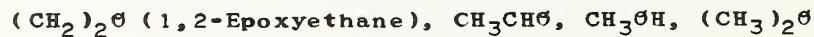
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CH_4 , C_2H_6

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X60 - 75

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$(\text{C}_5\text{H}_5)_2\text{Fe}$ (Bis(cyclopentadienyl)iron), PH_3 , NH_3 , $(\text{iso}-\text{C}_3\text{H}_7)_2\theta$, trans- $\text{CH}_3\text{N}=\text{NCH}_3$, CH_3NH_2 , H_2S

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SiH_4 , C_2H_2

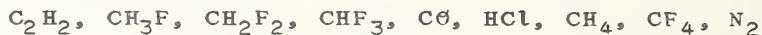
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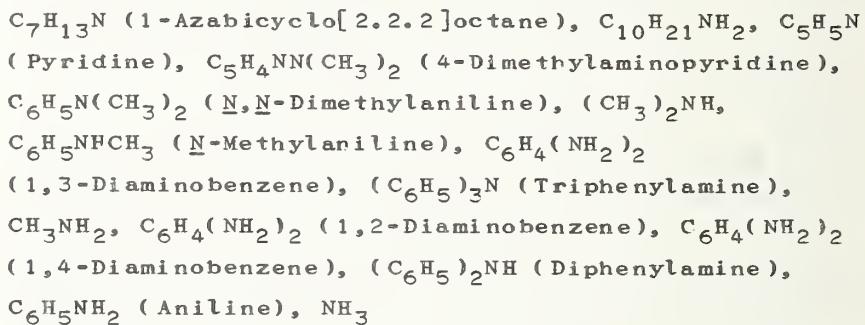
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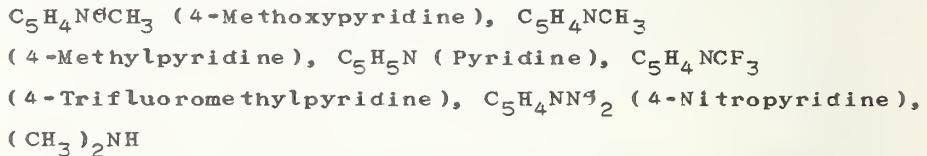
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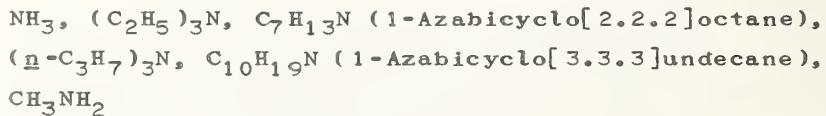
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D₂, Ar

X68 - 73

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SiH₄

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NF₃, HCl, CH₄

X72 - 72

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B₃H₆N₃ (Borazine), PH₃, CH₂=C=CH₂, CH₃C≡CH₃, NH₃

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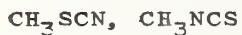
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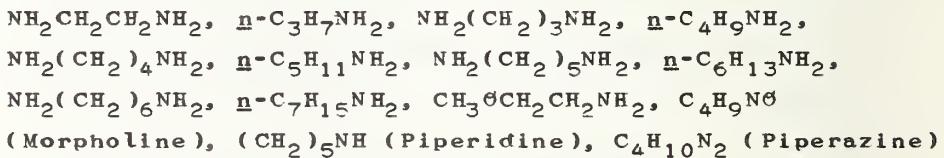
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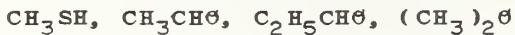
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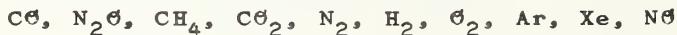
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SF₆

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X81 - 75

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CF₂, CH₃CN, CH₃CH₃O, CH₃O⁺H, AsH₃, HCH₃O, HCN, H₂O

X82 - 71

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(CH₃)₂CO, iso-C₄H₈, iso-C₃H₇O⁺H, NH₃, CH₂=CO

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CH₄, C₂H₆

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C₃H₈, C₂H₆

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HCOSH, CH_3SH , $\text{C}_2\text{H}_5\text{SH}$, HCOSH CH_3 , CH_3COSH , HCOSH C_2H_5 ,
 $\text{CH}_3\text{COSHCH}_3$, $\text{CH}_3\text{COSH}\text{C}_2\text{H}_5$, $(\text{CH}_3)_2\text{C}\theta$, $\text{C}_2\text{H}_5\text{COSHCH}_3$, $(\text{C}_2\text{H}_5)_2\text{C}\theta$,
 $\text{CH}_3\text{COSHSC}_2\text{H}_5$, $\text{CH}_3\text{COSHCH}_2\text{CH}_2\text{CH}_3$, $\text{CH}_3\text{COSHCH}_2\text{CH}_2\text{CH}_3$, $(\text{n-C}_4\text{H}_9)_2\theta$,
 $(\text{n-C}_4\text{H}_9)_2\text{S}$, $\text{ClCOSH}\text{C}_2\text{H}_5$

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trans- $\text{CH}_3\text{N}=\text{NCH}_3$, $\text{CHF}_2\text{CH}_2\text{NH}_2$, NH_3

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H_2 , Kr

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C_2H_6 , $\text{C}\theta$, CH_4 , $\text{N}_2\theta$, C_2H_4

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C₃H₈

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C₂H₆, C₃H₈

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AsH₃, PH₃, H₂S, CH₃CH=CH₂, CH₃O⁺H, CH₃Cl

X94 - 75 Kim, J. K., Theard, L. P., and Huntress, W. T., Jr., Proton Transfer Reactions from H₃⁺ Ions to N₂, O₂, and CO Molecules, *Chem. Phys. Letters* 32, 610 (1975).

O₂, H₂

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H₂, CH₄, CO, N₂, C₂H₆, N₂O

X96 - 72 Kasper, S. F., and Franklin, J. L., Ion-Molecule Reactions in the System CO₂-CH₄, *J. Chem. Phys.* 56, 1156 (1972).

CO₂, CH₄

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Kr, Xe, O₂, NO, H₂O, CH₄

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$(CH_3)_2\theta$, $(CH_3)_2CO$, $CH_3CH\theta$, $(CD_3)_2\theta$, $(CH_2)_2\theta$ (1,2-Epoxy-ethane)

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X100 - 72 Dixon, D. A., Holtz, D., and Beauchamp, J. L., Acidity, Basicity, and Gas-Phase Ion Chemistry of Hydrogen Selenide by Ion Cyclotron Resonance Spectroscopy, *Inorg. Chem.* 11, 960 (1972).

H_2Se , AsH_3 , H_2S , HCN , $H_2\theta$

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$C_6H_{10}\theta$ (Cyclohexanone)

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$(C_6H_5CH=CH)_2CO$ (1,5-Diphenyl-1,4-pentadien-3-one), $C_5H_2\theta_2(CH_3)_2$ (2,6-Dimethyl-4-pyrone), $C_{27}H_{44}\theta$ (4-Cholesten-3-one), $C_{27}H_{44}\theta$ (5-Cholesten-3-one), NH_3

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Kr, CH₄

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H₂O

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C₅H₅N (Pyridine), (CH₂)₅NH (Piperidine), (CH₂)₂NH (Ethylenimine), (CH₃)₂NH, CH₃CH=NC₂H₅, (C₂H₅)₂NH, (CH₃)₃N, (CH₂)₃NH (Trimethylenimine), (CH₂)₂NCH₃ (N-Methylethylenimine), C₂H₅NH₂, CH₃NH₂, C₃H₅N (1-Azabicyclo[1.1.0]butane), CH₃CN, C₂H₅CN, CH₃O₂H, (CH₂)₂O (1,2-Epoxyethane), (CH₃)₂O, (C₂H₅)₂O, (CF₂)₃O (1,3-Epoxypropane), (CH₃)₂CO, H₂O

X107 - 74 Staley, R. H., and Beauchamp, J. L., Relationship of Nitrogen Lone Pair Interactions to Thermodynamic Parameters Associated with Amine Basicities, *J. Am. Chem. Soc.* 96, 1604 (1974).

(CH₃)₃N, (C₂H₅)₃N, C₇H₁₃N (1-Azabicyclo[2.2.2]octane), C₆H₁₂N₂ (1,4-Diazabicyclo[2.2.2]octane), NH₃

X108 - 65 Waddington, T. C., Lattice Energies of Phosphonium Bromide and Iodide and the Proton Affinity of Phosphine, *Trans. Faraday Soc.* 61, 2652 (1965).

PH₃

X109 - 55 Wendlandt, W., Proton Affinity of Phosphine in the Phosphonium Halides, *Science* 122, 831 (1955).

PH₃

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NH_3

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NH_3 , $\text{H}_2\Theta$

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NH_3

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$\text{H}_2\Theta$, $\text{CH}_3\Theta\text{H}$, $\text{C}_2\text{H}_5\Theta\text{F}$, $n\text{-C}_4\text{H}_9\Theta\text{H}$

X114 - 59 Vetchinkin, S. I., Pshenichnov, E. A., and Sokolov, N. D., The Effect of the Hydrogen Bond on the Energy of the Ionic Lattice of Ammonium Chloride and Estimation of the Proton Affinity of an Ammonia Molecule, Zh. Fiz. Khim. 33, 1269 (1959).

NH_3

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NH_3

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C_2H_6 , C_3H_8 , C_4H_{10}

Y1 - 63 Van Raalte, D., and Harrison, A. G., Energetics and

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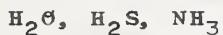
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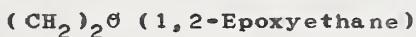
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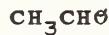


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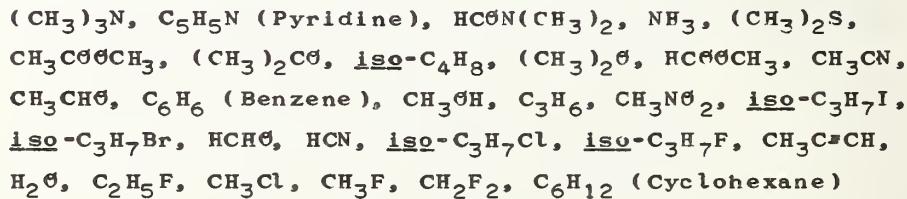
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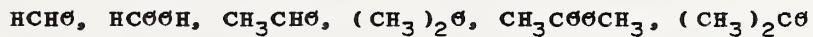
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CH₃CN

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(CH₂)₂NH

(Fthylenimine)

X99-73, X106-75

C₂H₅NH₂

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(CH₃)₂NH

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C₂H₅CN

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(CH₂)₂NCH₃

(N-Methylmethylenimine)

X106-75

(CH₂)₃NH

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n-C₃H₇NH₂

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iso-C₃H₇NH₂

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$(CH_2)_5NC_4H_7$
(N-(2-Methyl-1-propenyl)piperidine) 03-75

$(CH_2)_5NC_4H_9$
(N-Isobutylpiperidine) 03-75

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$(CH_2)_4NC_6H_9$
(N-(1-Cyclohexenyl)pyrrolidine) 03-75

$(CH_2)_4NC_6H_{11}$
(N-Cyclohexylpyrrolidine) 03-75

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$n-C_{10}H_{21}NH_2$ X64-72

$(CH_2)_5NC_6H_9$
(N-(1-Cyclohexenyl)piperidine) 03-75

$(CH_2)_5NC_6H_{11}$
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C6

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C6₂

X6-71, X7-73, X28-70, X44-75, X78-75, X96-72

N6

X6-71, X78-75, X97-65

N₂O

X6-71, X7-73, X78-75, X89-73, X95-74

LiOH

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HCHO

X3-70, X12-69, X16-75, X24-71, X27-65, X34-73,
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CH₃OH

X3-70, X11-58, X12-69, X16-75, X21-74, X24-71,
X27-65, X34-73, X35-68, X40-72, X45-72,
X46-72, X49-73, X51-74, X56-70, X81-75,
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CH₂=CH

X34-73, X82-71

CH₃CH₂O

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X37-70, X49-73, X56-70, X62-70, X77-75,
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(CH₂)₂O
(1,2-Epoxyethane)

X24-71, X56-70, X98-72, X106-75, Y7-69

C₂H₅OH

X11-58, X18-68, X24-71, X34-73, X49-73,
X113-55, Y8-66

(CH₃)₂O

X12-69, X24-71, X27-65, X34-73, X45-72, X51-74
X56-70, X59-75, X77-75, X98-72, X106-75,
O1-75, O4-75

(CD ₃) ₂ O	X98-72
C ₂ H ₅ CHO	X24-71, X49-73, X77-75, X85-73, Y8-66
(CH ₃) ₂ CO	X3-70, X5-69, X12-69, X24-71, X27-65, X34-73, X35-68, X37-70, X41-72, X49-73, X62-70, X82-71, X85-73, X98-72, X106-75, O1-75, O4-75
(CH ₂) ₃ O	
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C ₆ H ₁₀ O	
(Cyclohexanone)	X101-75
(<u>iso</u> -C ₃ H ₇) ₂ O	X52-74, X60-75
(n-C ₄ H ₉) ₂ O	X85-73
(C ₆ H ₅ CH=CH) ₂ CO	
(1,5-Diphenyl-1,4-pentadien-3-one)	X102-72

C₂₇H₄₄O

(4-Cholesten-3-one)

X102-72

C₂₇H₄₄O

(5-Cholesten-3-one)

X102-72

HC(O)H

X1-72, X12-69, X27-65, X32-74, X34-73,
X45-72, X46-72, X85-73, Y2-64, Y8-66, O4-75

CH₃C(O)H

X27-65, X34-73, X85-73, Y2-64, Y8-66, Y10-62

HC(O)CH₃

X34-73, X80-74, X85-73, O1-75

C₂H₅C(O)H

Y2-64, Y8-66

HC(O)C₂H₅

X34-73, X85-73

CH₃C(O)CH₃

X34-73, X85-73, O1-75, O4-75

HC(O)CH₂CH₂CH₃

X34-73

CH₃C(O)C₂H₅

X34-73, X85-73

C₂H₅C(O)CH₃

X34-73

CH₃C(O)CH₂CH₂CH₃

X34-73, X85-73

C₅H₂O₂(CH₃)₂

(2,6-Dimethyl-4-pyrone)

X102-72

(CH₃O)₂CO

X59-75

CH₃C(O)NH₂

X68-73

HC(O)N(CH₃)₂

O1-75

CH₃OCH₂CH₂NH₂

X76-73

C₄H₉NO

(Morpholine)

X76-73, O3-75

C₅H₄NOC₂H₅

(4-Methoxypyridine)

X65-72

$C_6H_4(NH_2)OCH_3$
(2-Methoxyaniline) X68-73

$C_4H_8NHC_4H_7$
(N-(2-Methyl-1-propenyl)morpholine) 03-75

$C_4H_8NHC_4H_9$
(N-Isobutylmorpholine) 03-75

$C_4H_8NHC_6H_9$
(N-(1-Cyclohexenyl)morpholine) 03-75

$C_4H_8NHC_6H_{11}$
(N-Cyclohexylmorpholine) 03-75

$C_4H_3N_2O$
(2-Hydroxy-1,3-diazine) X33-75

$C_4H_5N_3O$
(Cytosine) X33-75

$C_5H_4N_4O$
(Hypoxanthine) X33-75

$C_5H_5N_5O$
(Guanine) X33-75

$C_6H_7N_5O$
(8-Methylguanine) X33-75

$CH_3N_2O_2$ X31-70, X49-73, Q1-75

$C_2H_5N_2O_2$ X49-73

$C_4H_4N_2O_2$
(Uracil) X33-75

$C_5H_4NNO_2$
(4-Nitropyridine) X65-72

$C_5H_6N_2O_2$
(Thymine) X33-75

$C_2H_5NO_2$

X31-70, X49-73

$C_5H_3N_4C_5H_9O_4$

(9- β -D-Ribofuranosylpurine) X33-75

$C_5H_4N_5C_5H_9O_4$

(Adenosine) X33-75

$C_5H_5N_2O_2C_5H_9O_3$

(Thymidine) X33-75

$C_4H_4N_3O_2C_5H_9O_4$

(Cytidine) X33-75

$C_5H_4N_5O_2C_8H_{13}O_4$

(2',3'-O-Isopropylidene guanosine) X33-75

$C_4H_3N_2O_2C_5H_9O_4$

(Uridine) X33-75

$C_4H_5N_2O_2C_5H_9O_4$

(5,6-Dihydrouridine) X33-75

$C_4H_3N_2O_2C_8H_{13}O_4$

(2',3'-O-Isopropylidene uridine) X33-75

F Q6-74

HF X24-71, X44-75

BF₃ X30-75

CF₂ X81-75

CF₄ X6-71, X63-74

NF₃ X71-71

BHF₂ X30-75

CH₃F X29-72, X54-70, X63-74, O1-75

C₂H₃F X16-75

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CH ₂ =CF ₂	X16-75
<u>c</u> <u>i</u> <u>s</u> -CHF=CHF	X16-75
<u>t</u> <u>r</u> <u>a</u> <u>n</u> <u>s</u> -CHF=CHF	X16-75
CHF ₃	X63-74
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(CH ₃) ₃ P	X38-70, X52-74
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C_2H_5Cl	X29-72, X54-70
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C₂H₅I

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